Supporting Information for:

Conformational analysis of 2,2'–bithiophene revisited: the Maximum Entropy method applied to large sets of H–H and ^{13}C–H partially averaged dipolar couplings

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ij	F	RMS
11-12	3.67	159.22
11-13	3.36	150.88
12-13	3.35	120.67
11-14	3.34	93.25
11-15	3.07	17.90
11-16	2.94	1.64
12-15	...	...
12-16	...	...
13-16	2.88	0.53 ; 2.22
1-12	...	...
1-13	...	...
1-14	...	...
1-15	...	...
1-16	...	...
2-13	2.52	2.10
2-14	2.31	2.07
2-15	2.29	2.00
2-16	...	...
3-14	...	...
3-15	...	...
3-16	...	...
4-11	...	...
4-14	...	...
4-15	...	...
4-16	...	...

TABLE I: Values of the minimum of the functional F and the root mean square (RMS) error after every addition of the dipolar couplings ij for the case of 2,2'–bithiophene dissolved in the nematic solvent I52. In correspondence of the dipolar coupling 13-16 two are the values of RMS reported: the first calculated considering only the H–H dipolar couplings; the second considering all the listed dipolar couplings. The symbol ... in correspondence of the columns F and RMS means that the minimum of F is unstable and the RMS is growing considerably and irregularly if the corresponding dipolar coupling is added to the previous retained data.

ij	$\lambda_{ij} \times 10$
11-12	-0.123
11-13	0.441
12-13	-0.055
11-14	-0.007
11-15	0.283
11-16	0.373
13-16	0.769

TABLE II: The parameters λ_{ij} in Eqs. 3 and 4 of the main text for the case of 2,2'–bithiophene dissolved in the nematic solvent I52, considering only the indicated seven, within the ME context linearly independent, H–H dipolar couplings in the minimization of the functional F.

ij	D_{exp} (Hz)	D_{cal}(Hz)	$100 \times \frac{D_{cal}-D_{exp}}{D_{exp}}$
11-12	-2261.91	-2261.98	0.003
11-13	-117.85	-117.84	-0.005
12-13	766.04	766.02	-0.002
11-14	-774.29	-774.55	0.033
11-15	-201.26	-201.29	0.017
11-16	-236.01	-236.01	0.000
12-15	-89.77	-88.31	-1.620
12-16	-89.96	-90.03	0.077
13-16	-75.04	-75.04	0.000
1-12	-243.7	-248.6	2.01
1-13	-216.9	-222.1	2.42
1-14	-160.9	-158.0	-1.82
1-15	-101.5	-101.1	-0.41
1-16	-88.3	-90.3	2.30
2-13	-111.1	-110.6	-0.46
2-14	-144.5	-151.6	4.93
2-15	-56.3	-56.1	-0.27
2-16	-58.4	-58.7	0.53
3-14	-80.1	-79.1	-1.23
3-15	-33.4	-32.9	-1.39
3-16	-31.8	-32.1	1.07
4-11	-25.4	-25.9	1.93
4-14	-89.2	-88.6	-0.64
4-15	-33.4	-32.9	-1.47
4-16	-28.9	-28.1	-2.83

TABLE III: Experimental (D_{exp}) and calculated (D_{cal}) dipolar couplings, together with their percentage difference, of 2,2'–bithiophene dissolved in the nematic solvent I52. The calculated dipolar couplings have been obtained by adopting the procedure described in the main text, considering only the sub–set of seven, within the ME context linearly independent, H–H dipolar couplings in the minimization of the functional F.

ij	F	RMS
11-12	3.23	199.28
11-13	3.22	194.48
12-13	3.20	140.70
11-14	3.19	108.12
11-15	2.78	24.91
11-16	2.53	1.29
12-15	...	...
12-16	...	...
13-16	2.42	1.20 ; 2.78
1-12	...	...
1-13	...	...
1-14	...	...
1-15	...	...
1-16	...	...
2-13	...	...
2-14	1.50	2.13
2-15	...	...
2-16	...	...
3-14	...	...
3-15	...	...
3-16	...	...
4-11	...	...
4-14	...	...
4-15	...	...
4-16	...	...

TABLE IV: Values of the minimum of the functional F and the root mean square (RMS) error after every addition of the dipolar couplings ij for the case of 2,2'–bithiophene dissolved in the nematic solvent ZLI1132. In correspondence of the dipolar coupling 13-16 two are the values of RMS reported: the first calculated considering only the H–H dipolar couplings; the second considering all the listed dipolar couplings. The symbol ... in correspondence of the columns F and RMS means that the minimum of F is unstable and the RMS is growing considerably and irregularly if the corresponding dipolar coupling is added to the previous retained data.

ij	$\lambda_{ij} \times 10$
11-12	-0.197
11-13	0.704
12-13	-0.088
11-14	-0.012
11-15	0.459
11-16	0.580
13-16	1.228

TABLE V: The parameters λ_{ij} in Eqs. 3 and 4 of the main text for the case of 2,2'–bithiophene dissolved in the nematic solvent ZLI1132, considering only the indicated seven, within the ME context linearly independent, H–H dipolar couplings in the minimization of the functional F.

ij	D_{exp} (Hz)	D_{cal}(Hz)	$100 \times \frac{D_{cal}-D_{exp}}{D_{exp}}$
11-12	-2742.66	-2740.32	-0.085
11-13	-194.74	-194.18	-0.289
12-13	768.22	768.02	-0.025
11-14	-876.63	-874.97	-0.189
11-15	-219.12	-219.17	0.021
11-16	-267.12	-267.12	0.000
12-15	-99.97	-97.81	-2.158
12-16	-104.39	-104.09	-0.287
13-16	-91.24	-91.16	-0.089
1-12	-267.9	-270.1	0.82
1-13	-267.4	-273.6	2.34
1-14	-152.1	-150.1	-1.29
1-15	-113.3	-112.2	-0.98
1-16	-107.8	-109.0	1.15
2-13	-158.2	-158.7	0.30
2-14	-157.0	-165.6	5.49
2-15	-60.2	-61.7	2.50
2-16	-68.0	-68.4	0.61
3-14	-88.1	-83.2	-5.53
3-15	-36.8	-36.7	-0.35
3-16	-37.9	-37.7	-0.49
4-11	-60.9	-61.4	0.76
4-14	-98.7	-97.5	-1.22
4-15	-41.7	-37.6	-9.92
4-16	-33.9	-33.9	0.00

TABLE VI: Experimental (D_{exp}) and calculated (D_{cal}) dipolar couplings, together with their percentage difference, of 2,2'–bithiophene dissolved in the nematic solvent ZLI1132. The calculated dipolar couplings have been obtained by adopting the procedure described in the main text, considering only the sub–set of seven, within the ME context linearly independent, H–H dipolar couplings in the minimization of the functional F.

ij	$\lambda_{ij} \times 10$
11-12	-0.012
11-13	1.215
12-13	-0.157
11-14	-0.024
11-15	2.638
11-16	1.170
13-16	5.209
2-14	-1.343
2-15	-2.199
2-16	-5.523

TABLE VII: The parameters λ_{ij} in Eqs. 3 and 4 of the main text for the case of 2,2'–bithiophene dissolved in the nematic solvent I52, considering the indicated, within the ME context linearly independent, H–H and ^{13}C–H dipolar couplings in the minimization of the functional F.

ij	D_{exp} (Hz)	D_{cal}(Hz)	$100 \times \frac{D_{cal}-D_{exp}}{D_{exp}}$
11-12	-2261.91	-2260.59	-0.058
11-13	-117.85	-118.16	0.263
12-13	766.04	768.41	0.310
11-14	-774.29	-773.45	-0.108
11-15	-201.26	-201.45	0.094
11-16	-236.01	-236.25	0.103
12-15	-89.77	-88.47	-1.444
12-16	-89.96	-89.69	-0.295
13-16	-75.04	-75.20	0.213
1-12	-243.7	-247.6	1.61
1-13	-216.9	-222.1	2.39
1-14	-160.9	-156.2	-2.89
1-15	-101.5	-100.8	-0.72
1-16	-88.3	-90.3	2.30
2-13	-111.1	-110.7	-0.31
2-14	-144.5	-144.3	-0.10
2-15	-56.3	-56.3	-0.00
2-16	-58.4	-58.5	0.26
3-14	-80.1	-78.6	-1.84
3-15	-33.4	-32.9	-1.37
3-16	-31.8	-32.0	0.80
4-11	-25.4	-26.0	2.52
4-14	-89.2	-88.6	-0.64
4-15	-33.4	-32.8	-1.87
4-16	-28.9	-28.1	-2.72

TABLE VIII: Experimental (D_{exp}) and calculated (D_{cal}) dipolar couplings, together with their percentage difference, of 2,2'–bithiophene dissolved in the nematic solvent I52. The calculated dipolar couplings have been obtained by adopting the procedure described in the main text, considering the, within the ME context linearly independent, H–H and ^{13}C–H dipolar couplings in the minimization of the functional F.

ij	$\lambda_{ij} \times 10$
11-12	-0.453
11-13	3.164
12-13	-0.386
11-14	-0.063
11-15	5.011
11-16	1.336
13-16	-7.033
2-14	-2.996

TABLE IX: The parameters λ_{ij} in Eqs. 3 and 4 of the main text for the case of 2,2'–bithiophene dissolved in the nematic solvent ZLI1132, considering only the indicated, within the ME context linearly independent, H–H and ^{13}C–H dipolar couplings in the minimization of the functional F.

ij	D_{exp} (Hz)	D_{cal}(Hz)	$100 \times \frac{D_{cal}-D_{exp}}{D_{exp}}$
11-12	-2742.66	-2743.86	0.044
11-13	-194.74	-195.04	0.157
12-13	768.22	768.22	0.000
11-14	-876.63	-875.88	-0.086
11-15	-219.12	-218.90	-0.101
11-16	-267.12	-267.15	0.012
12-15	-99.97	-98.13	-1.840
12-16	-104.39	-104.04	-0.332
13-16	-91.24	-91.27	0.034
1-12	-267.9	-269.9	0.75
1-13	-267.4	-274.1	2.50
1-14	-152.1	-149.5	-1.73
1-15	-113.3	-112.2	-1.00
1-16	-107.8	-109.2	1.27
2-13	-158.2	-159.2	0.63
2-14	-157.0	-156.8	-0.12
2-15	-60.2	-62.0	2.90
2-16	-68.0	-68.5	0.68
3-14	-88.1	-84.9	-3.62
3-15	-36.8	-36.8	-0.14
3-16	-37.9	-37.7	-0.44
4-11	-60.9	-61.8	1.45
4-14	-98.7	-97.4	-1.29
4-15	-41.7	-37.5	-10.01
4-16	-33.9	-33.9	0.00

TABLE X: Experimental (D_{exp}) and calculated (D_{cal}) dipolar couplings, together with their percentage difference, of 2,2'–bithiophene dissolved in the nematic solvent ZLI1132. The calculated dipolar couplings have been obtained by adopting the procedure described in the main text, considering the, within the ME context linearly independent, H–H and ^{13}C–H dipolar couplings in the minimization of the functional F.